



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:54 PM UTC

PDB ID : 1E8Z / pdb_00001e8z
Title : Structure determinants of phosphoinositide 3-kinase inhibition by wortmannin, LY294002, quercetin, myricetin and staurosporine
Authors : Walker, E.H.; Pacold, M.E.; Perisic, O.; Stephens, L.; Hawkins, P.T.; Wymann, M.P.; Williams, R.L.
Deposited on : 2000-10-03
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

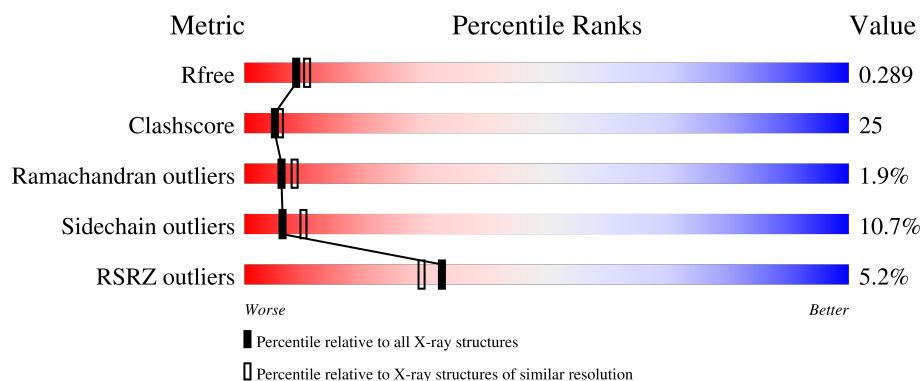
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	5% 47% 33% 7% 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6876 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

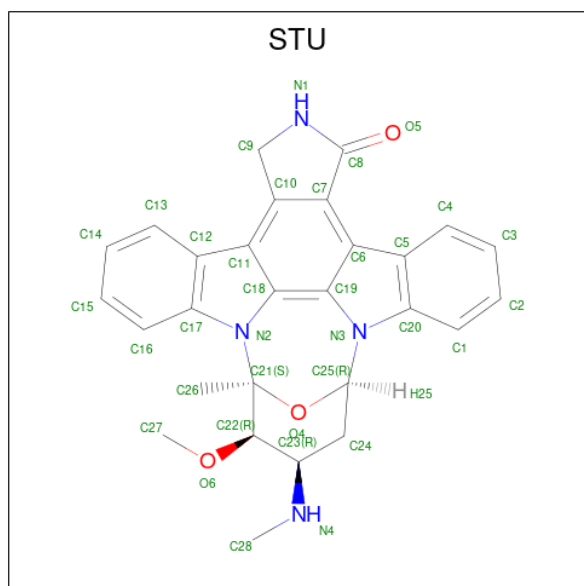
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	839	6801	4367	1162	1237	35	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	PRO	cloning artifact	UNP P48736
A	505	ALA	ARG	conflict	UNP P48736

- Molecule 2 is STAUROSPORINE (CCD ID: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	35	28	4	3	0	0

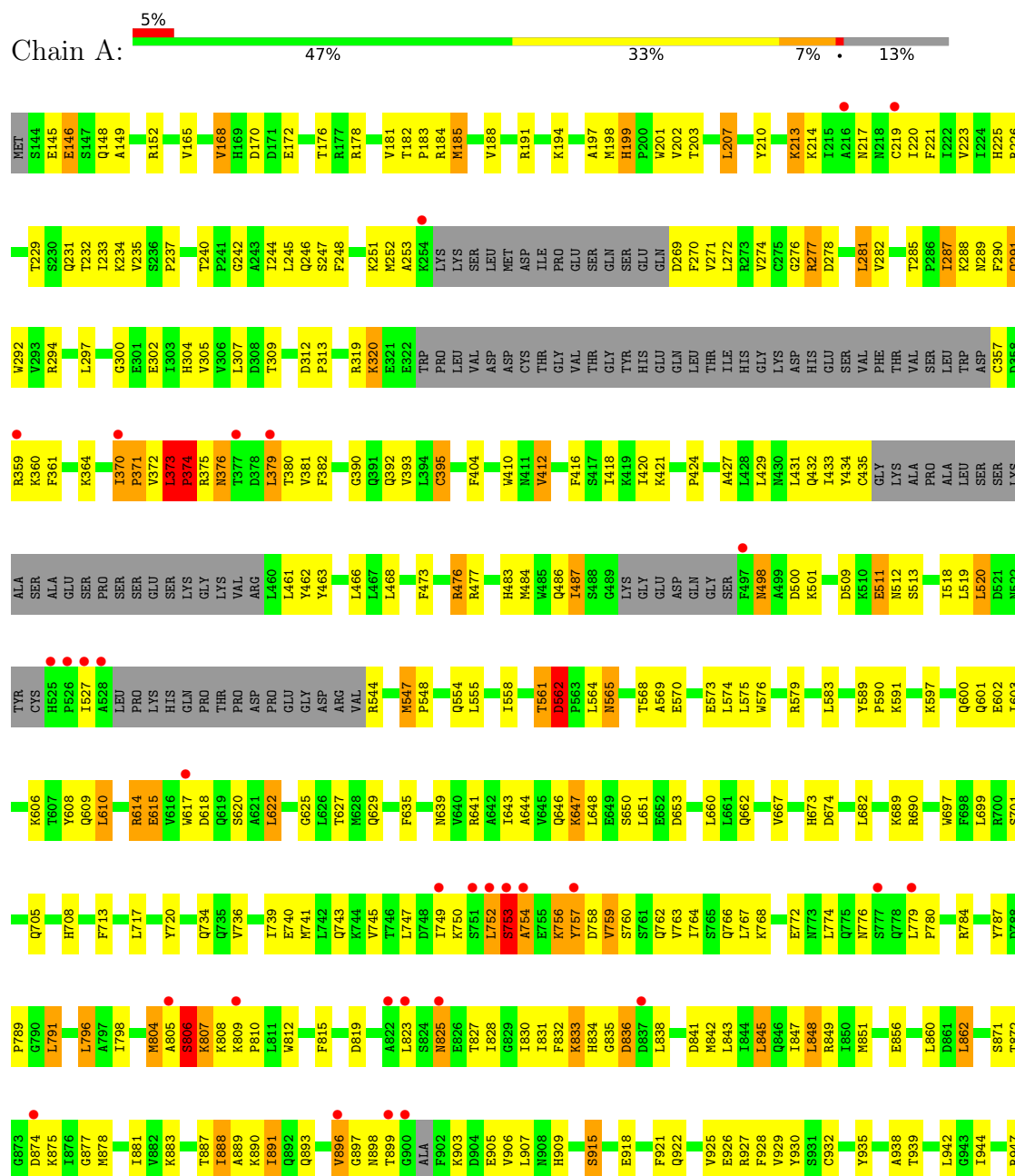
- Molecule 3 is water.

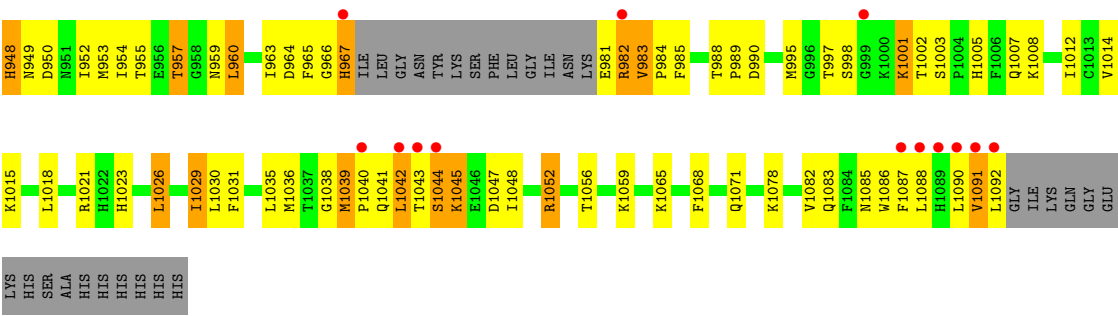
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.49Å 66.99Å 104.11Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	60.84 – 2.40 60.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.9 (60.84-2.40) 87.9 (60.84-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.42Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.291 0.232 , 0.289	Depositor DCC
R_{free} test set	1935 reflections (5.89%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6876	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: STU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	2/6946 (0.0%)	1.04	19/9393 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	MET	SD-CE	6.02	1.94	1.79
1	A	953	MET	SD-CE	5.04	1.92	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	MET	CA-C-N	6.62	126.59	119.78
1	A	547	MET	C-N-CA	6.62	126.59	119.78
1	A	253	ALA	N-CA-C	-6.52	105.18	113.01
1	A	565	ASN	CA-C-N	6.19	126.13	119.76
1	A	565	ASN	C-N-CA	6.19	126.13	119.76
1	A	614	ARG	N-CA-C	6.12	117.61	111.07
1	A	511	GLU	N-CA-C	6.08	117.99	111.36
1	A	562	ASP	CA-C-N	6.06	126.22	119.32
1	A	562	ASP	C-N-CA	6.06	126.22	119.32
1	A	930	TYR	N-CA-C	5.53	117.11	111.14
1	A	660	LEU	N-CA-C	5.35	117.53	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	891	ILE	N-CA-C	-5.20	105.46	110.72
1	A	199	HIS	N-CA-C	5.19	121.29	109.81
1	A	412	VAL	N-CA-C	5.17	115.92	108.48
1	A	915	SER	CA-C-N	5.16	125.46	119.47
1	A	915	SER	C-N-CA	5.16	125.46	119.47
1	A	948	HIS	CA-C-N	5.07	127.78	120.38
1	A	948	HIS	C-N-CA	5.07	127.78	120.38
1	A	888	ILE	N-CA-C	-5.06	105.61	110.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	720	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6801	0	6845	341	0
2	A	35	0	26	0	0
3	A	40	0	0	2	0
All	All	6876	0	6871	341	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (341) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.41	1.01
1:A:149:ALA:HA	1:A:152:ARG:HD3	1.43	1.00
1:A:381:VAL:HG23	1:A:435:CYS:HB3	1.44	0.98
1:A:981:GLU:N	1:A:982:ARG:HH21	1.62	0.97
1:A:750:LYS:HE2	1:A:809:LYS:H	1.30	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:THR:HG21	1:A:950:ASP:HA	1.50	0.93
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.53	0.90
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.18	0.90
1:A:240:THR:HG22	1:A:242:GLY:H	1.39	0.87
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.56	0.85
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.74	0.85
1:A:981:GLU:C	1:A:982:ARG:HE	1.84	0.85
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.57	0.84
1:A:202:VAL:HG12	1:A:203:THR:N	1.93	0.83
1:A:860:LEU:HD11	1:A:1015:LYS:HG2	1.63	0.81
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.62	0.81
1:A:887:THR:HG22	1:A:889:ALA:H	1.46	0.80
1:A:379:LEU:HD13	1:A:380:THR:H	1.48	0.79
1:A:217:ASN:ND2	1:A:219:CYS:HB3	1.98	0.79
1:A:750:LYS:HA	1:A:809:LYS:HG3	1.63	0.79
1:A:836:ASP:O	1:A:875:LYS:HA	1.83	0.78
1:A:561:THR:HG22	1:A:591:LYS:NZ	2.00	0.77
1:A:750:LYS:HE2	1:A:809:LYS:N	2.00	0.77
1:A:380:THR:O	1:A:435:CYS:HB2	1.86	0.76
1:A:935:TYR:O	1:A:939:THR:HG22	1.87	0.75
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.69	0.75
1:A:1044:SER:O	1:A:1045:LYS:HG3	1.86	0.74
1:A:887:THR:CG2	1:A:950:ASP:HA	2.17	0.74
1:A:568:THR:HG22	1:A:570:GLU:H	1.52	0.74
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.03	0.73
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.70	0.73
1:A:379:LEU:HD13	1:A:380:THR:N	2.05	0.71
1:A:807:LYS:HD2	1:A:808:LYS:H	1.55	0.70
1:A:1039:MET:HE2	1:A:1039:MET:N	2.07	0.69
1:A:965:PHE:O	1:A:967:HIS:N	2.26	0.69
1:A:245:LEU:O	1:A:248:PHE:HB3	1.92	0.68
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.73	0.68
1:A:371:PRO:HG2	1:A:511:GLU:O	1.93	0.68
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.29	0.68
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.41	0.68
1:A:791:LEU:HD12	1:A:828:ILE:HD11	1.76	0.67
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.76	0.67
1:A:277:ARG:CZ	1:A:791:LEU:HD23	2.23	0.67
1:A:202:VAL:CG1	1:A:203:THR:N	2.57	0.67
1:A:486:GLN:HG2	1:A:487:ILE:H	1.58	0.67
1:A:825:ASN:H	1:A:825:ASN:HD22	1.42	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:GLU:N	1:A:982:ARG:NH2	2.40	0.67
1:A:625:GLY:O	1:A:629:GLN:HG3	1.96	0.66
1:A:182:THR:HB	1:A:183:PRO:HD3	1.77	0.66
1:A:213:LYS:NZ	1:A:214:LYS:HB2	2.11	0.66
1:A:558:ILE:O	1:A:561:THR:HB	1.96	0.66
1:A:848:LEU:HA	1:A:851:MET:HE2	1.78	0.66
1:A:202:VAL:HG12	1:A:203:THR:H	1.59	0.66
1:A:617:TRP:CE2	1:A:643:ILE:HD12	2.31	0.66
1:A:202:VAL:HG13	1:A:289:ASN:O	1.96	0.65
1:A:597:LYS:HB2	1:A:603:ILE:HD13	1.76	0.65
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.79	0.65
1:A:888:ILE:HD13	1:A:952:ILE:HG22	1.78	0.65
1:A:1042:LEU:HD13	1:A:1042:LEU:H	1.60	0.65
1:A:202:VAL:CG1	1:A:203:THR:H	2.10	0.64
1:A:1002:THR:HG22	1:A:1003:SER:H	1.63	0.64
1:A:375:ARG:HG2	1:A:376:ASN:H	1.61	0.64
1:A:1043:THR:C	1:A:1045:LYS:H	2.04	0.64
1:A:373:LEU:H	1:A:374:PRO:HD2	1.63	0.64
1:A:569:ALA:O	1:A:573:GLU:HG3	1.98	0.64
1:A:833:LYS:HG3	1:A:834:HIS:N	2.13	0.64
1:A:270:PHE:HB3	1:A:307:LEU:HD11	1.79	0.63
1:A:825:ASN:H	1:A:825:ASN:ND2	1.97	0.62
1:A:498:ASN:HB3	1:A:1041:GLN:NE2	2.13	0.62
1:A:373:LEU:H	1:A:374:PRO:CD	2.13	0.62
1:A:561:THR:HG22	1:A:591:LYS:HZ1	1.63	0.61
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.40	0.61
1:A:181:VAL:O	1:A:185:MET:HG3	2.00	0.61
1:A:395:CYS:HB2	1:A:418:ILE:HD12	1.82	0.61
1:A:149:ALA:O	1:A:152:ARG:HB2	2.01	0.61
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.30	0.60
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.31	0.60
1:A:851:MET:HE1	1:A:938:ALA:CB	2.28	0.59
1:A:148:GLN:O	1:A:152:ARG:HG3	2.02	0.59
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.68	0.59
1:A:983:VAL:HG23	1:A:1082:VAL:HG21	1.85	0.59
1:A:832:PHE:HE1	1:A:878:MET:HE2	1.68	0.58
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.85	0.58
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.30	0.58
1:A:807:LYS:HD2	1:A:807:LYS:N	2.19	0.58
1:A:221:PHE:CE2	1:A:234:LYS:HG2	2.38	0.57
1:A:287:ILE:HD12	1:A:288:LYS:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLN:OE1	1:A:501:LYS:NZ	2.37	0.57
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.26	0.57
1:A:804:MET:HB2	1:A:810:PRO:HB2	1.85	0.57
1:A:291:GLN:HA	1:A:291:GLN:OE1	2.03	0.57
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.40	0.57
1:A:690:ARG:NH1	1:A:789:PRO:HG2	2.20	0.57
1:A:836:ASP:H	1:A:875:LYS:HB3	1.69	0.57
1:A:1042:LEU:HD13	1:A:1042:LEU:N	2.20	0.57
1:A:168:VAL:HG13	1:A:170:ASP:H	1.70	0.57
1:A:874:ASP:O	1:A:875:LYS:HB2	2.03	0.57
1:A:561:THR:HG22	1:A:591:LYS:HZ2	1.70	0.57
1:A:277:ARG:NH2	1:A:791:LEU:HD23	2.20	0.57
1:A:1036:MET:HA	1:A:1042:LEU:HD11	1.86	0.57
1:A:768:LYS:O	1:A:772:GLU:HG2	2.04	0.56
1:A:370:ILE:HD12	1:A:372:VAL:O	2.05	0.56
1:A:170:ASP:OD1	1:A:170:ASP:C	2.48	0.56
1:A:734:GLN:HA	1:A:734:GLN:HE21	1.69	0.56
1:A:739:ILE:O	1:A:743:GLN:HG3	2.06	0.56
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.05	0.56
1:A:845:LEU:O	1:A:849:ARG:HG3	2.06	0.56
1:A:1038:GLY:C	1:A:1039:MET:HE2	2.31	0.56
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.70	0.55
1:A:165:VAL:HG12	1:A:165:VAL:O	2.06	0.55
1:A:1002:THR:HG22	1:A:1003:SER:N	2.21	0.55
1:A:758:ASP:CG	1:A:759:VAL:H	2.13	0.55
1:A:787:TYR:OH	1:A:830:ILE:HG12	2.05	0.55
1:A:220:ILE:HD12	1:A:287:ILE:HD13	1.87	0.55
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.37	0.55
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.54	0.55
1:A:835:GLY:HA2	1:A:875:LYS:HE3	1.90	0.54
1:A:1052:ARG:HG2	1:A:1052:ARG:HH11	1.72	0.54
1:A:745:VAL:HG21	1:A:774:LEU:HD11	1.90	0.54
1:A:791:LEU:HD12	1:A:828:ILE:CD1	2.37	0.54
1:A:246:GLN:C	1:A:248:PHE:H	2.16	0.54
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.37	0.54
1:A:410:TRP:O	1:A:412:VAL:HG23	2.07	0.54
1:A:662:GLN:NE2	1:A:1030:LEU:HD22	2.22	0.54
1:A:207:LEU:HA	1:A:294:ARG:NH1	2.23	0.54
1:A:988:THR:HB	1:A:989:PRO:CD	2.38	0.54
1:A:370:ILE:HD13	1:A:371:PRO:N	2.23	0.54
1:A:149:ALA:HA	1:A:152:ARG:HH11	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HG3	1:A:178:ARG:HH11	1.73	0.53
1:A:653:ASP:OD1	3:A:2021:HOH:O	2.19	0.53
1:A:743:GLN:O	1:A:747:LEU:HG	2.09	0.53
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.24	0.53
1:A:561:THR:HG23	1:A:565:ASN:HB3	1.91	0.53
1:A:805:ALA:O	1:A:806:SER:O	2.27	0.53
1:A:233:ILE:N	1:A:233:ILE:HD12	2.22	0.53
1:A:753:SER:HB2	1:A:809:LYS:NZ	2.24	0.52
1:A:235:VAL:HG11	1:A:244:ILE:HD11	1.92	0.52
1:A:804:MET:HE3	1:A:810:PRO:HB2	1.92	0.52
1:A:1044:SER:C	1:A:1045:LYS:HG3	2.34	0.52
1:A:697:TRP:HH2	1:A:739:ILE:HD13	1.75	0.52
1:A:483:HIS:HD2	3:A:2013:HOH:O	1.92	0.52
1:A:361:PHE:HB2	1:A:420:ILE:CD1	2.39	0.52
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.10	0.52
1:A:240:THR:HG22	1:A:242:GLY:N	2.17	0.52
1:A:949:ASN:N	1:A:1083:GLN:HE22	1.97	0.52
1:A:606:LYS:HA	1:A:609:GLN:OE1	2.11	0.51
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.92	0.51
1:A:947:ARG:NH2	1:A:963:ILE:O	2.44	0.51
1:A:905:GLU:HB3	1:A:909:HIS:NE2	2.25	0.51
1:A:251:LYS:HB3	1:A:252:MET:SD	2.51	0.51
1:A:276:GLY:HA2	1:A:819:ASP:CG	2.35	0.51
1:A:359:ARG:HG3	1:A:360:LYS:N	2.26	0.51
1:A:622:LEU:HD21	1:A:651:LEU:HD21	1.93	0.51
1:A:219:CYS:SG	1:A:234:LYS:HB3	2.51	0.51
1:A:763:VAL:HG13	1:A:764:ILE:N	2.25	0.51
1:A:887:THR:HG21	1:A:950:ASP:OD1	2.11	0.51
1:A:699:LEU:HD22	1:A:713:PHE:HD2	1.76	0.50
1:A:831:ILE:HG13	1:A:881:ILE:HD11	1.93	0.50
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.25	0.50
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.94	0.50
1:A:375:ARG:HG2	1:A:376:ASN:N	2.25	0.50
1:A:997:THR:HG23	1:A:1001:LYS:HB3	1.94	0.50
1:A:749:ILE:HG12	1:A:767:LEU:HD23	1.93	0.50
1:A:963:ILE:HD12	1:A:964:ASP:OD1	2.10	0.50
1:A:390:GLY:C	1:A:392:GLN:H	2.20	0.50
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.92	0.50
1:A:568:THR:HG22	1:A:569:ALA:N	2.25	0.50
1:A:997:THR:HG22	1:A:998:SER:N	2.26	0.50
1:A:600:GLN:CB	1:A:603:ILE:HD12	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:VAL:CG1	1:A:985:PHE:O	2.59	0.50
1:A:435:CYS:SG	1:A:461:LEU:CD1	3.00	0.49
1:A:848:LEU:HD12	1:A:851:MET:CE	2.42	0.49
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.94	0.49
1:A:562:ASP:OD1	1:A:1052:ARG:NH1	2.45	0.49
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.76	0.49
1:A:278:ASP:OD1	1:A:784:ARG:NH2	2.45	0.49
1:A:739:ILE:HG22	1:A:878:MET:CE	2.42	0.49
1:A:760:SER:O	1:A:763:VAL:HG12	2.12	0.49
1:A:198:MET:HE3	1:A:282:VAL:HG21	1.95	0.49
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.13	0.49
1:A:1086:TRP:HH2	1:A:1090:LEU:HB2	1.78	0.49
1:A:232:THR:C	1:A:233:ILE:HD12	2.37	0.49
1:A:893:GLN:HA	1:A:897:GLY:O	2.13	0.49
1:A:807:LYS:HD2	1:A:808:LYS:N	2.27	0.48
1:A:955:THR:OG1	1:A:957:THR:HG22	2.12	0.48
1:A:270:PHE:HB3	1:A:307:LEU:CD1	2.41	0.48
1:A:373:LEU:HD11	1:A:404:PHE:O	2.12	0.48
1:A:739:ILE:HG13	1:A:740:GLU:N	2.27	0.48
1:A:932:CYS:HA	1:A:960:LEU:HD22	1.94	0.48
1:A:197:ALA:HA	1:A:689:LYS:HE3	1.95	0.48
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.14	0.48
1:A:1043:THR:HB	1:A:1047:ASP:H	1.78	0.48
1:A:836:ASP:N	1:A:875:LYS:HB3	2.29	0.48
1:A:896:VAL:CG2	1:A:903:LYS:HG3	2.43	0.48
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	1.95	0.48
1:A:149:ALA:CB	1:A:152:ARG:HH11	2.27	0.48
1:A:1086:TRP:O	1:A:1087:PHE:CD1	2.67	0.48
1:A:1052:ARG:HG2	1:A:1052:ARG:NH1	2.28	0.47
1:A:433:ILE:HG13	1:A:484:MET:HE1	1.96	0.47
1:A:244:ILE:HA	1:A:247:SER:OG	2.14	0.47
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.79	0.47
1:A:862:LEU:CD2	1:A:862:LEU:N	2.77	0.47
1:A:997:THR:HG22	1:A:998:SER:H	1.79	0.47
1:A:395:CYS:HB2	1:A:418:ILE:CD1	2.43	0.47
1:A:600:GLN:HG3	1:A:603:ILE:HD12	1.96	0.47
1:A:1085:ASN:O	1:A:1087:PHE:N	2.47	0.47
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.96	0.47
1:A:568:THR:CG2	1:A:569:ALA:N	2.77	0.47
1:A:948:HIS:NE2	1:A:950:ASP:HB2	2.30	0.47
1:A:643:ILE:HG13	1:A:644:ALA:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:TRP:C	1:A:1087:PHE:CD1	2.93	0.47
1:A:213:LYS:HZ3	1:A:214:LYS:HB2	1.79	0.47
1:A:983:VAL:CG2	1:A:1082:VAL:HG21	2.44	0.47
1:A:213:LYS:HD3	1:A:214:LYS:N	2.30	0.47
1:A:667:VAL:O	1:A:667:VAL:HG12	2.14	0.47
1:A:210:TYR:OH	1:A:856:GLU:HG3	2.15	0.46
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.80	0.46
1:A:796:LEU:HG	1:A:815:PHE:CE2	2.50	0.46
1:A:983:VAL:HG13	1:A:984:PRO:HD2	1.97	0.46
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.15	0.46
1:A:1021:ARG:NH2	1:A:1056:THR:HG23	2.31	0.46
1:A:188:VAL:O	1:A:191:ARG:HG2	2.16	0.46
1:A:832:PHE:CE1	1:A:878:MET:HE2	2.48	0.46
1:A:954:ILE:HA	1:A:959:ASN:O	2.14	0.46
1:A:576:TRP:O	1:A:579:ARG:HG2	2.14	0.46
1:A:1021:ARG:NE	1:A:1056:THR:CG2	2.78	0.46
1:A:602:GLU:O	1:A:606:LYS:HG3	2.16	0.46
1:A:758:ASP:CG	1:A:759:VAL:N	2.73	0.46
1:A:762:GLN:O	1:A:766:GLN:HG3	2.15	0.46
1:A:246:GLN:C	1:A:248:PHE:N	2.73	0.46
1:A:361:PHE:C	1:A:361:PHE:CD2	2.93	0.46
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	1.97	0.45
1:A:1021:ARG:HH21	1:A:1056:THR:HG23	1.81	0.45
1:A:772:GLU:OE2	1:A:798:ILE:HG21	2.15	0.45
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.98	0.45
1:A:320:LYS:H	1:A:320:LYS:HG3	1.39	0.45
1:A:424:PRO:HG2	1:A:427:ALA:HB2	1.97	0.45
1:A:1043:THR:C	1:A:1045:LYS:N	2.70	0.45
1:A:172:GLU:CD	1:A:673:HIS:CD2	2.95	0.45
1:A:1008:LYS:HG3	1:A:1012:ILE:HD11	1.98	0.45
1:A:217:ASN:HD22	1:A:219:CYS:HB3	1.76	0.45
1:A:841:ASP:O	1:A:845:LEU:HD22	2.17	0.45
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.51	0.45
1:A:390:GLY:C	1:A:392:GLN:N	2.74	0.44
1:A:983:VAL:CG2	1:A:1078:LYS:HG2	2.47	0.44
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.99	0.44
1:A:281:LEU:CD2	1:A:305:VAL:HG21	2.48	0.44
1:A:848:LEU:HD12	1:A:851:MET:HE1	1.98	0.44
1:A:1001:LYS:HG3	1:A:1002:THR:H	1.82	0.44
1:A:364:LYS:O	1:A:518:ILE:HA	2.18	0.44
1:A:807:LYS:N	1:A:807:LYS:CD	2.79	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLN:CD	1:A:252:MET:HE1	2.43	0.44
1:A:891:ILE:HG22	1:A:906:VAL:CG1	2.46	0.44
1:A:921:PHE:O	1:A:925:VAL:HG23	2.18	0.44
1:A:614:ARG:CZ	1:A:643:ILE:HG22	2.48	0.43
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.99	0.43
1:A:431:LEU:O	1:A:463:TYR:HA	2.18	0.43
1:A:1001:LYS:NZ	1:A:1001:LYS:HB2	2.33	0.43
1:A:1014:VAL:HG11	1:A:1065:LYS:HD2	2.01	0.43
1:A:750:LYS:HA	1:A:809:LYS:CG	2.42	0.43
1:A:756:LYS:HE3	1:A:757:TYR:N	2.34	0.43
1:A:929:VAL:HG22	1:A:995:MET:HG2	2.00	0.43
1:A:622:LEU:HD22	1:A:650:SER:OG	2.19	0.43
1:A:146:GLU:HB3	1:A:319:ARG:HH22	1.84	0.43
1:A:498:ASN:HB3	1:A:1041:GLN:HE22	1.82	0.43
1:A:955:THR:C	1:A:957:THR:N	2.76	0.43
1:A:312:ASP:HA	1:A:313:PRO:HD2	1.89	0.43
1:A:804:MET:CE	1:A:812:TRP:HB2	2.37	0.43
1:A:825:ASN:ND2	1:A:825:ASN:N	2.66	0.43
1:A:214:LYS:NZ	1:A:297:LEU:HA	2.34	0.43
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.49	0.43
1:A:1043:THR:O	1:A:1045:LYS:N	2.50	0.43
1:A:701:SER:O	1:A:705:GLN:HG3	2.19	0.42
1:A:1021:ARG:NE	1:A:1056:THR:HG23	2.33	0.42
1:A:357:CYS:SG	1:A:359:ARG:HB3	2.59	0.42
1:A:635:PHE:O	1:A:641:ARG:HD2	2.19	0.42
1:A:752:LEU:O	1:A:753:SER:CB	2.65	0.42
1:A:1026:LEU:O	1:A:1026:LEU:HD22	2.18	0.42
1:A:745:VAL:CG2	1:A:774:LEU:HD11	2.49	0.42
1:A:935:TYR:O	1:A:939:THR:CG2	2.60	0.42
1:A:754:ALA:C	1:A:756:LYS:H	2.27	0.42
1:A:939:THR:OG1	1:A:944:ILE:HG13	2.20	0.42
1:A:995:MET:O	1:A:1005:HIS:HB2	2.19	0.42
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.49	0.42
1:A:382:PHE:CE1	1:A:434:TYR:HB2	2.55	0.42
1:A:774:LEU:C	1:A:776:ASN:H	2.28	0.42
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.24	0.42
1:A:620:SER:O	1:A:647:LYS:NZ	2.51	0.42
1:A:862:LEU:N	1:A:862:LEU:HD22	2.35	0.42
1:A:888:ILE:CG2	1:A:949:ASN:OD1	2.67	0.42
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.50	0.42
1:A:486:GLN:HG2	1:A:487:ILE:N	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.54	0.42
1:A:614:ARG:O	1:A:615:GLU:C	2.63	0.42
1:A:210:TYR:O	1:A:213:LYS:HD2	2.20	0.42
1:A:734:GLN:HE22	1:A:780:PRO:HB3	1.85	0.41
1:A:918:GLU:O	1:A:922:GLN:HG2	2.20	0.41
1:A:473:PHE:HB3	1:A:527:ILE:HD12	2.02	0.41
1:A:486:GLN:CG	1:A:487:ILE:H	2.31	0.41
1:A:547:MET:HA	1:A:548:PRO:HD3	1.81	0.41
1:A:736:VAL:O	1:A:740:GLU:HB2	2.20	0.41
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.56	0.41
1:A:627:THR:HG21	1:A:648:LEU:HD21	2.02	0.41
1:A:890:LYS:HE3	1:A:890:LYS:HB2	1.80	0.41
1:A:928:PHE:HE2	1:A:995:MET:HE2	1.85	0.41
1:A:420:ILE:HD13	1:A:420:ILE:HA	1.90	0.41
1:A:477:ARG:HA	1:A:520:LEU:HB3	2.03	0.41
1:A:739:ILE:HG22	1:A:878:MET:HE3	2.03	0.41
1:A:149:ALA:CA	1:A:152:ARG:HH11	2.33	0.41
1:A:589:TYR:O	1:A:590:PRO:C	2.63	0.41
1:A:1031:PHE:O	1:A:1035:LEU:HG	2.19	0.41
1:A:214:LYS:HZ3	1:A:297:LEU:HA	1.86	0.41
1:A:278:ASP:OD1	1:A:784:ARG:CZ	2.69	0.41
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.88	0.41
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.28	0.41
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.51	0.41
1:A:842:MET:HE2	1:A:871:SER:HB2	2.03	0.41
1:A:237:PRO:HA	1:A:287:ILE:HD11	2.03	0.41
1:A:617:TRP:CZ2	1:A:643:ILE:HD12	2.56	0.41
1:A:928:PHE:CE2	1:A:995:MET:HE2	2.55	0.41
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.86	0.41
1:A:184:ARG:HH11	1:A:184:ARG:HB2	1.85	0.41
1:A:242:GLY:O	1:A:245:LEU:HB2	2.20	0.41
1:A:357:CYS:O	1:A:421:LYS:HB2	2.20	0.41
1:A:509:ASP:O	1:A:513:SER:OG	2.37	0.41
1:A:614:ARG:HD3	1:A:646:GLN:HE22	1.85	0.41
1:A:804:MET:HB2	1:A:804:MET:HE3	1.77	0.41
1:A:988:THR:HB	1:A:989:PRO:HD2	2.02	0.41
1:A:1021:ARG:C	1:A:1023:HIS:N	2.77	0.41
1:A:373:LEU:N	1:A:374:PRO:CD	2.81	0.41
1:A:750:LYS:CE	1:A:808:LYS:HB3	2.50	0.41
1:A:223:VAL:HB	1:A:304:HIS:CD2	2.56	0.40
1:A:739:ILE:CG1	1:A:740:GLU:N	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:THR:HG22	1:A:888:ILE:N	2.36	0.40
1:A:462:TYR:HB3	1:A:484:MET:HE2	2.03	0.40
1:A:618:ASP:OD1	1:A:646:GLN:OE1	2.39	0.40
1:A:806:SER:HB2	1:A:810:PRO:HG2	2.02	0.40
1:A:198:MET:O	1:A:199:HIS:C	2.64	0.40
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.22	0.40
1:A:896:VAL:HG22	1:A:903:LYS:HG3	2.02	0.40
1:A:181:VAL:HG12	1:A:185:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	821/966 (85%)	741 (90%)	64 (8%)	16 (2%)	6 8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	615	GLU
1	A	753	SER
1	A	806	SER
1	A	898	ASN
1	A	966	GLY
1	A	1040	PRO
1	A	1088	LEU
1	A	373	LEU
1	A	754	ALA
1	A	1091	VAL
1	A	374	PRO
1	A	1044	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1045	LYS
1	A	371	PRO
1	A	759	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	754/864 (87%)	673 (89%)	81 (11%)	6 10

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	168	VAL
1	A	185	MET
1	A	194	LYS
1	A	207	LEU
1	A	213	LYS
1	A	226	ARG
1	A	229	THR
1	A	269	ASP
1	A	271	VAL
1	A	277	ARG
1	A	281	LEU
1	A	287	ILE
1	A	291	GLN
1	A	309	THR
1	A	320	LYS
1	A	370	ILE
1	A	373	LEU
1	A	374	PRO
1	A	379	LEU
1	A	393	VAL
1	A	395	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	476	ARG
1	A	487	ILE
1	A	498	ASN
1	A	512	ASN
1	A	520	LEU
1	A	544	ARG
1	A	554	GLN
1	A	555	LEU
1	A	561	THR
1	A	562	ASP
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	622	LEU
1	A	647	LYS
1	A	682	LEU
1	A	717	LEU
1	A	752	LEU
1	A	753	SER
1	A	756	LYS
1	A	757	TYR
1	A	779	LEU
1	A	791	LEU
1	A	796	LEU
1	A	804	MET
1	A	806	SER
1	A	807	LYS
1	A	823	LEU
1	A	825	ASN
1	A	827	THR
1	A	833	LYS
1	A	836	ASP
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	862	LEU
1	A	883	LYS
1	A	896	VAL
1	A	899	THR
1	A	907	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	915	SER
1	A	926	GLU
1	A	957	THR
1	A	960	LEU
1	A	967	HIS
1	A	982	ARG
1	A	983	VAL
1	A	1001	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1039	MET
1	A	1042	LEU
1	A	1052	ARG
1	A	1059	LYS
1	A	1091	VAL
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	225	HIS
1	A	304	HIS
1	A	391	GLN
1	A	396	GLN
1	A	483	HIS
1	A	486	GLN
1	A	565	ASN
1	A	639	ASN
1	A	646	GLN
1	A	662	GLN
1	A	708	HIS
1	A	734	GLN
1	A	737	GLN
1	A	766	GLN
1	A	773	ASN
1	A	825	ASN
1	A	959	ASN
1	A	1041	GLN
1	A	1083	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	STU	A	3001	-	39,42,42	3.56	27 (69%)	50,68,68	2.23	7 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STU	A	3001	-	-	0/4/42/42	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	STU	C25-N3	8.45	1.52	1.45
2	A	3001	STU	C16-C17	6.02	1.49	1.39
2	A	3001	STU	C13-C12	5.44	1.48	1.40
2	A	3001	STU	C17-N2	5.33	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	STU	C8-N1	-5.22	1.31	1.35
2	A	3001	STU	C6-C7	5.21	1.50	1.40
2	A	3001	STU	C22-C23	5.11	1.58	1.53
2	A	3001	STU	C26-C21	4.86	1.56	1.51
2	A	3001	STU	C1-C20	4.71	1.46	1.39
2	A	3001	STU	C11-C10	4.52	1.49	1.40
2	A	3001	STU	C4-C5	4.37	1.46	1.40
2	A	3001	STU	C24-C25	3.96	1.59	1.51
2	A	3001	STU	C19-C18	3.90	1.49	1.40
2	A	3001	STU	C18-N2	-3.82	1.35	1.40
2	A	3001	STU	O6-C22	3.41	1.48	1.42
2	A	3001	STU	C12-C11	-3.28	1.39	1.46
2	A	3001	STU	C19-N3	-3.06	1.34	1.39
2	A	3001	STU	C6-C19	2.99	1.47	1.41
2	A	3001	STU	C14-C13	2.76	1.43	1.38
2	A	3001	STU	C5-C6	-2.70	1.40	1.46
2	A	3001	STU	C2-C1	2.67	1.43	1.38
2	A	3001	STU	C11-C18	2.56	1.46	1.41
2	A	3001	STU	C7-C10	2.52	1.43	1.39
2	A	3001	STU	C15-C16	2.47	1.43	1.38
2	A	3001	STU	C20-N3	2.42	1.43	1.40
2	A	3001	STU	C3-C4	2.08	1.42	1.38
2	A	3001	STU	C24-C23	2.02	1.56	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	STU	C9-C10-C7	-8.50	106.76	109.88
2	A	3001	STU	C28-N4-C23	7.37	123.19	114.39
2	A	3001	STU	C9-C10-C11	6.34	133.54	128.73
2	A	3001	STU	C16-C17-C12	-3.43	117.58	121.59
2	A	3001	STU	C11-C10-C7	-2.35	119.70	121.25
2	A	3001	STU	C12-C17-N2	2.20	110.39	108.94
2	A	3001	STU	C18-N2-C17	-2.18	104.73	107.37

There are no chirality outliers.

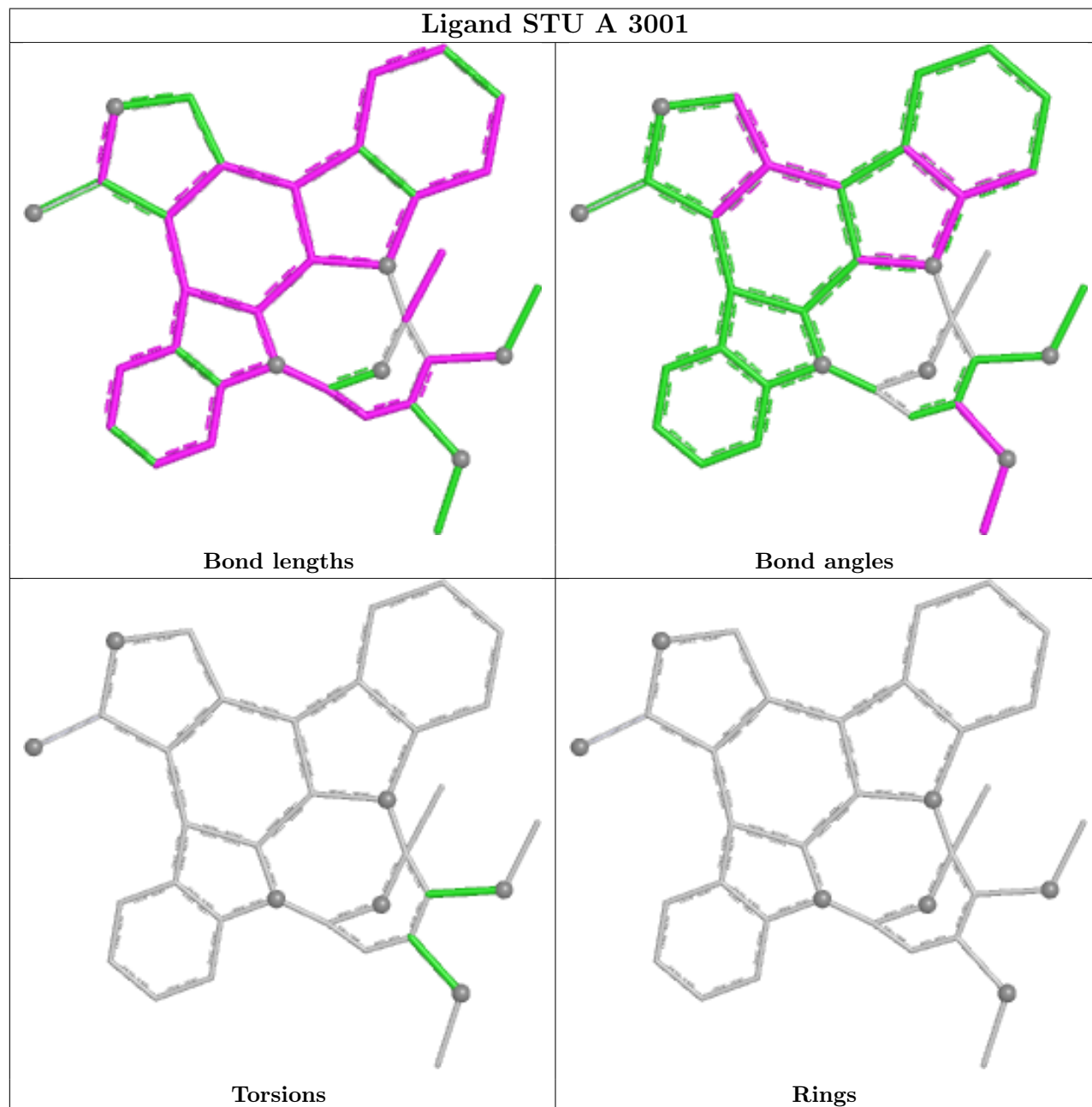
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	839/966 (86%)	0.34	44 (5%) 33 29	25, 51, 94, 119	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	900	GLY	5.0
1	A	751	SER	4.8
1	A	823	LEU	4.7
1	A	1092	LEU	4.4
1	A	1088	LEU	4.2
1	A	528	ALA	4.1
1	A	1089	HIS	4.0
1	A	379	LEU	3.9
1	A	752	LEU	3.8
1	A	1090	LEU	3.8
1	A	1087	PHE	3.7
1	A	899	THR	3.6
1	A	525	HIS	3.1
1	A	1042	LEU	3.1
1	A	1091	VAL	3.1
1	A	753	SER	3.0
1	A	1044	SER	3.0
1	A	874	ASP	2.8
1	A	1040	PRO	2.7
1	A	967	HIS	2.7
1	A	779	LEU	2.7
1	A	617	TRP	2.7
1	A	777	SER	2.6
1	A	527	ILE	2.6
1	A	216	ALA	2.6
1	A	896	VAL	2.5
1	A	809	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	837	ASP	2.4
1	A	757	TYR	2.4
1	A	377	THR	2.4
1	A	370	ILE	2.4
1	A	497	PHE	2.4
1	A	982	ARG	2.3
1	A	805	ALA	2.3
1	A	219	CYS	2.3
1	A	526	PRO	2.3
1	A	825	ASN	2.2
1	A	254	LYS	2.2
1	A	999	GLY	2.2
1	A	749	ILE	2.2
1	A	359	ARG	2.2
1	A	1043	THR	2.1
1	A	754	ALA	2.1
1	A	822	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

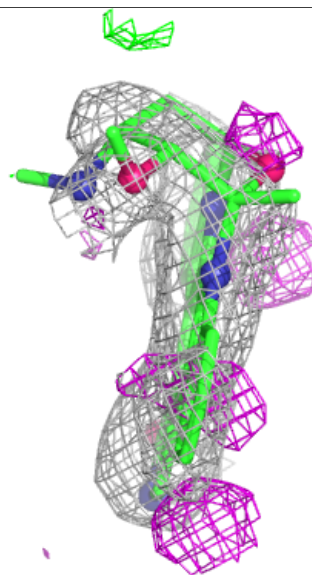
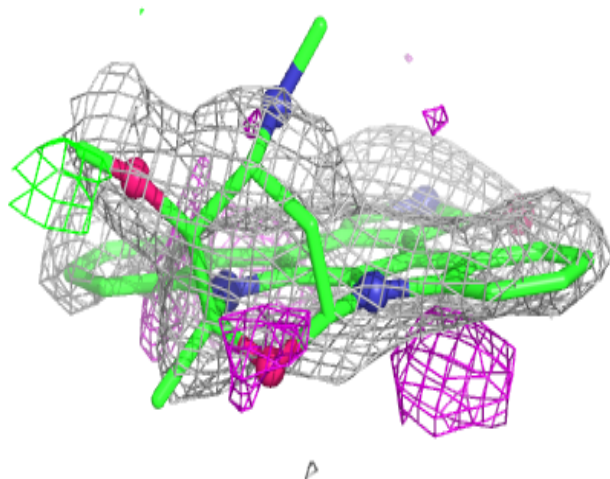
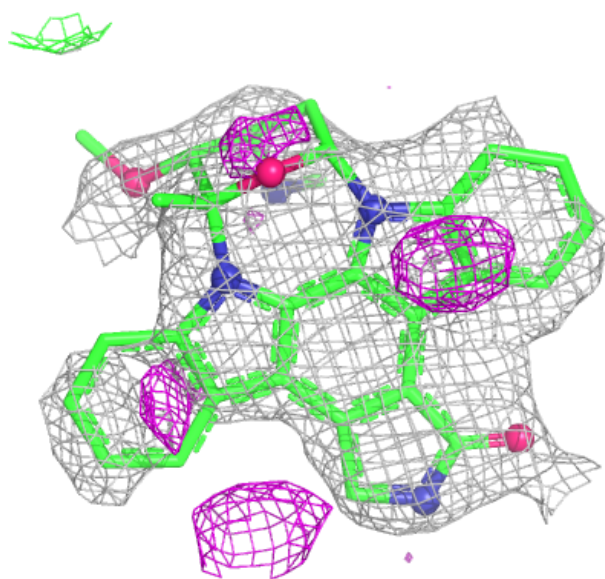
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	STU	A	3001	35/35	0.76	0.17	74,78,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around STU A 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.